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Mathematical prediction of the Jatropha curcas L. plant yield: comparing Multiple Linear Regression and Artificial Neural Network Multilayer Perceptron models.

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Abstract. The aim of this study was to predict *Jatropha curcas* plant yield through an Artificial Neural Network (ANN) Multi-Layer Perceptron (MLP) model. The predictive ability of the developed model was tested against the Multiple Linear Regression (MLR) using performance indexes. According to the performance indexes the use of ANN-MLP model improved *Jatropha curcas* plant yield prediction comparatively to MLR model.

Key words: Yield; *Jatropha curcas* plant; Multiple Linear Regression; Artificial Neural Networks-Multi-Layer Perceptron; Modeling.
AMS 2010 Mathematics Subject Classification Objects : 62J05; 90B10; 92B20.

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Résumé (Abstract in French) L'objectif de cette étude était de prédire le rendement de la plante *Jatropha curcas* avec un modèle de réseau de neurones artificiels (ANN) perceptron multicouches (MLP). La capacité prédictive du modèle développé a été testée par rapport à la régression linéaire multiple (MLR) en utilisant des indices de performance. Selon les indices de performance, l'utilisation du modèle ANN-MLP a amélioré la prédiction de rendement de la plante *Jatropha curcas* comparativement au modèle MLR.

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Introduction

Bio-energy species such as *Jatropha curcas* plant yield prediction is a matter of importance in most of the countries in West Africa. The socio-economic importance of *Jatropha curcas* plant lies in the ability of the seed to produce easily convertible oil in biodiesel (Francis et al., 2005). It is an alternative to fossil fuel in the current crisis of fossil fuels accompanied by a number of increasingly high car (Prasad et al., 2000). Various different approaches like statistical, mechanistic, deterministic, stochastic, dynamic, static, simulations are used for assessing and predicting crop growth and yield (Bannayan et al., 2003). Some are based on growing models of plant, thus by predicting status of plant at harvesting time, yield prediction can be performed. In statistical approaches, most of the researchers have employed regression models for prediction purposes in various disciplines. Due to the nature of linear relationship in the parameters, regression models may not provide accurate predictions in some complex situations such as non-linear data and extreme values data (Çakır et al., 2014). The artificial neural network (ANN) can find nonlinear management conditions (Liu et al., 2001). Unlike generalized linear models (GLM, McCullagh and Nelder (1983)), it is not necessary to specify the type of relationship between covariates and response variables as for instance as linear combination. This makes artificial neural networks a valuable statistical tool (Günther and Fritsch, 2010). One of the commonly used network type is Multi-Layer Perceptron (MLP) neural networks, where the number of inputs, the number of neurons in the hidden layers, the type of nonlinearity in the output of neurons can be chosen as desired (Çakır et al., 2014). Perceptron Multi-layer can approximate all booelienne function at condition that number of neural in hidden layer is appropriate (Günther and Fritsch, 2010). The MLP is one of the most widely used neural networks for approximation, classification and prediction problems (Parizeau, 2004). The ANN was used to predict wheat yield production (Çakır et al., 2014), surface ozone concentration (Sousa et al., 2007; Moustris et al., 2012), heavy metals soluble in surface water (El Badaoui et al., 2012), to model the river flows (Koffi et al.,

2014).
Gbèmavo et al. (2015) predicted the performance of *Jatropha curcas* plant according to agro-morphological parameters using multiple linear regressions after Box and Cox transformation (Box and Cox, 1964) to the adjustment of *Jatropha curcas* plant yield values to the requirements involved by the application of MLR analysis. This prediction approach makes it possible to circumvent the violation of the application conditions of the multiple linear regressions in particular the non-normality of the residuals but does not correct the nonlinearity between the dependent and independent variables. Measurements on *Jatropha curcas* plant individuals were used to test the validity of the established model. A coefficient of determination of 55% between the predicted and the quantified values in the field showed that the established model needs to be improved. Moreover, the value of λ after the transformation of Box and Cox is negative, which is not interesting because they lead to more compression of the high values. The main research question for this study is: Is the use of multilayer perceptron neural networks a better approach to predicting agricultural yields as a solution in the event of persistent nonlinearity between variables?

Materials and methods

The data used in this paper were extracted from a study by Gbèmavo et al. (2015). 60 *Jatropha curcas* plant trees randomly chosen from six townships in the three climatic zones of Benin, were selected in 2013. Data collected from each *Jatropha curcas* plant tree were: diameter at breast height (cm), total height (m), height at first branch, number of branch (primary, secondary and tertiary) and the yield (g/tree). The results of Pearson correlation between yield and the principal's components of morphometric characteristics of *Jatropha curcas* plant showed a significant relation between yield and morphometric characteristic of *Jatropha curcas* plant such as diameter at breast height, total height, number of branch (primary, secondary and tertiary). These variables were used for the prediction.

Statistic

The data was subdivided into two samples. The first sample constitutes of 75% random selection of the data and the second sample the rest (25%) of the data. The two predictive models, namely MLR and ANN-MLP, were applied to the 45 (75%) *Jatropha curcas* plant trees randomly selected sample of all the samples that formed the target group, learning a predictive model of the dependent variable. The remaining 25% of the samples were used to test the validity and performance of the prediction of these models.

MLR

The first step was to adjust *Jatropha curcas* plant yield values to the requirements of the application of MLR analysis (normality of residues, homogeneity of residues, independence of residues, null mean residues and linearity). Most of the assumptions of the MLR were not met. The Box and Cox transformation (Box and Cox, 1964) was applied to meet the normality of residues. The first model is in the form (eq. 1):

$$y = \alpha_0 + \alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_3 + \alpha_4 x_4 + \alpha_5 x_5 + \varepsilon \qquad \text{(eq. 1)}$$

where y is the response variable, α_0 is the intercept term, $\alpha = (\alpha_1, \ldots, \alpha_5)$ are the regression coefficients, $x = (x_1, \ldots, x_5)$ are the independent predictor variables, and ε is a residual error. x_1 = diameter at breast height, x_2 = number of primary branch, x_3 = number of secondary branch, x_4 = number of tertiary branch, x_5 = total height.

Nevertheless, in regression equations, the collinearity between the independent variables can lead to incorrect identification of the most important predictors (Thompson et al., 2001; Heo and Kim, 2004). For this purpose, a multicollinearity index namely variance inflation factor (VIF) was used (Hossain et al., 2010). According to Hossain et al. (2010), if $0 < VIF < 5$, there is no evidence of multicollinearity. If $5 \leq VIF \leq 10$, there is a moderate multicollinearity, and finally if $VIF > 10$, there is high multicollinearity between predictors. The obtained VIF values varied between 1.40 to 1.60, suggesting absence of multicollinearity problem of *Jatropha curcas* plant variables after transformation.

ANN-MLP

Before establishing Artificial Neural Network (ANN) Multilayer Perceptron model (MLP), the data were normalized to bring all values into the range $[0, 1]$ (unity-based normalization). The following equation were used to implement the unity-based normalization (eq. 2):

$$X_{i,\ \text{0 to 1}} = \frac{X_i - X_{min}}{X_{max} - X_{min}} \qquad \text{(eq. 2)}$$

where:
X_i = Each data point I;
X_{min} = The minima among all the data points;
X_{max} = The maxima among all the data points;
$X_{i,\ \text{0 to 1}}$ = The data point i normalized between 0 and 1.

The underlying structure of an MLP is a directed graph, i.e. it consists of vertices and directed edges, in this context called neurons and synapses (Günther and Fritsch, 2010). The neurons are organized in layers, which are usually fully connected by synapses. In neuralnet, a synapse can only connect to subsequent layers. The input layer consists of all covariates in separate neurons and the output layer consists of the response variables. The layers in between are referred to as hidden layers, as they are not directly observable. Input layer and hidden layers include a constant neuron relating to intercept synapses, i.e. synapses that are not directly influenced by any covariate. Perceptron Multi-layer can approximate all booelienne function at condition that number of neural in hidden layer is appropriate (Günther and Fritsch, 2010). The package *neuralnet* (Stefan and Guenther, 2016) which focuses on multi-layer perceptron (MLP, Bishop et al. (1995)), was used. *Neuralnet* includes the calculation of generalized weights ($\widetilde{w}_i$) as introduced by Intrator and Intrator (2001). The generalized weight $\widetilde{w}_i$ is defined as the contribution of the i^{th} covariate to the log-odds (eq. 3):

$$\widetilde{w}_i = \frac{\partial \log\left(\dfrac{o(x)}{1-o(x)}\right)}{\partial x_i} \qquad \text{(eq. 3)}$$

The generalized weight expresses the effect of each covariate x_i and thus has an analogous interpretation as the i^{th} regression parameter in regression models. However, the generalized weight depends on all other covariates. Its distribution indicates whether the effect of the covariate is linear since a small variance suggests a linear effect (Intrator and Intrator, 2001). Covariates have a nonlinear effect when the variance of their generalized weights is overall greater than zero.
The Artificial Neural Network was performing using two hidden layers. The equation from the input layer to the hidden layer is presented as follows (eq. 4):

$$\begin{cases} v_1 = a_0 + a_1x_1 + a_2x_2 + a_3x_3 + a_4x_4 + a_5x_5 \\ v_2 = b_0 + b_1x_1 + b_2x_2 + b_3x_3 + b_4x_4 + b_5x_5 \end{cases} \qquad \text{(eq. 4)}$$

where a_0 (or b_0) denotes the intercept, $a = (a1, \ldots, a5)$ $[b = (b1, \ldots, b5)]$ the vector consisting of all synaptic weights without the intercept, and $x = (x_1, \ldots, x_5)$ the vector of all covariates. x_1 = diameter at breast height, x_2 = number of primary branch, x_3 = number of secondary branch, x_4 = number of tertiary branch, x_5 = total height. Output equation of hidden layer is presented as follows (eq. 5):

$$\begin{cases} \mu_1 = g(v_1) = \dfrac{1}{1+e^{-v_1}} \\[2ex] \mu_2 = g(v_2) = \dfrac{1}{1+e^{-v_2}} \end{cases} \qquad \text{(eq. 5)}$$

The equation from hidden layer to the output layer is presented as follows (eq. 6):

$$z = c_0 + c_1\mu_1 + c_2\mu_2 \qquad \text{(eq. 6)}$$

The equation of output network (final equation) is presented as follows (eq. 7):

$$\hat{y} = g(z) = \frac{1}{1+e^{-z}} \qquad \text{(eq. 7)}$$

For the evaluation of the predicting performance of the developed model, appropriate statistical indices such as the coefficient of determination (R^2), the mean bias error (MBE), the root mean square error (RMSE) and the index of agreement (IA) were used (Moustris et al., 2012; Comrie, 1997; Willmott, 1982; Willmott et al., 1985; Walker et al., 1999; Kolehmainen et al., 2001; Dutot et al., 2007) (table 1).

Table 1: Performance indexes.

Indexes	**Formula**
Coefficient of determination (R^2)	$\dfrac{\left[\sum_{i=1}^{n}(y_i-\bar{y})(\hat{y}_i-\bar{\hat{y}})\right]^2}{\sum_{i=1}^{n}(y_i-\bar{y})^2\times\sum_{i=1}^{n}(\hat{y}_i-\bar{\hat{y}})^2}$
Root Mean Square Error (RMSE)	$\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i-\hat{y}_i)^2}$
Mean Bias Error (MBE)	$\frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i-y_i)$
Index of Agreement (IA)	$1-\dfrac{\left[\sum_{i=1}^{n}\lvert\hat{y}_i-y_i\rvert^2\right]}{\left[\sum_{i=1}^{n}\left(\lvert\hat{y}_i-\bar{y}_i\rvert-\lvert y_i-\bar{y}_i\rvert\right)^2\right]}$

y = observed values; $\bar{y}$ = mean of observed values; $\hat{y}$ = predicted values and $\bar{\hat{y}}$ = mean of predicted values.

The RMSE is a frequently used measure of the differences between the predicted values and the observed values. The RMSE was used as a single measure that indicates the ability of the model to predict and has the same units as the predicted value. The RMSE is always positive and a zero value is ideal. The MBE provides information on the long-term performance. A low MBE is desirable. Ideally a zero value of MBE should be obtained. A positive value gives the average amount of overestimation in the calculated and negative underestimate. The coefficient of determination is used in cases of statistical models, whose main purpose is the forecast of future outcomes on the basis of other related information. It is the proportion of the variability in a dataset that is accounted for by the statistical model. It provides a measure of how well future outcomes are likely to be predicted by the model. The coefficient of determination values range from zero to one ($0 \leq R^2 \leq 1$). The closer the value is to one, the better and more accurate is the prediction. The index of agreement is a dimension less measure with values between zero and one ($0 \leq IA \leq 1$). When IA = 0, there is no agreement between prediction and observation, while IA=1 denotes a perfect agreement between prediction and observation (Willmott, 1982). These performances indexes were computed using *tdr* package (Lamigueiro, 2015) for R^2, RMSE and MBE indexes and *hydroGOF* (Zambrano-Bigiarini, 2014) package for IA (also noted d) index. Data were analyzed in R-3.6.1 software (R Core Team, 2019).

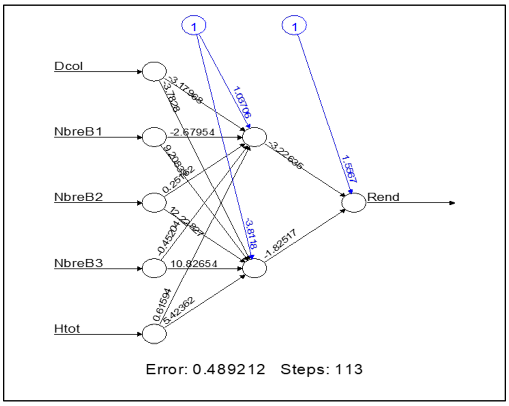
Results and discussion

Jatropha curcas plant yield modeling

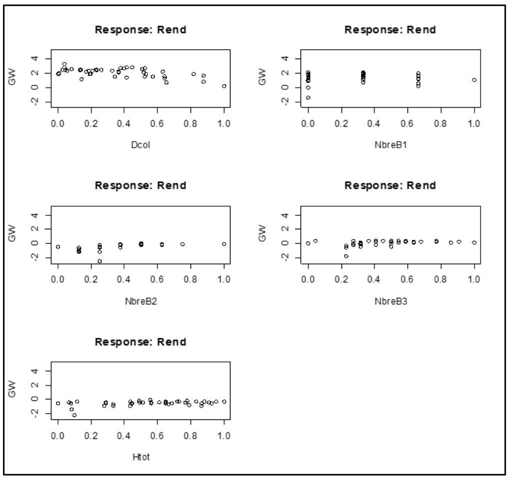
The estimated MLR model is significant ($F = 2.88$; $P = 0.025$) and was:

$$y' = 0.14 - 8.8\times10^{-4}x_1 - 5.9\times10^{-3}x_2 + 8.4\times10^{-4}x_3 - 6.7\times10^{-4}x_4 - 8.7\times10^{-4}x_5 \quad \text{with } y' = y^{-0.36}$$

The training process of ANN-MLP model needed 113 steps until all absolute partial derivatives of the error function were smaller than 0.00865 (the default threshold). The estimated weights range from -3.78 to 12.22. For instance, the intercepts of the



(a) Plot of a trained neural network including trained synaptic weights and basic information about the training process



(b) Plots of generalized weights ($\widetilde{w}_i$) with respect to each covariate

Fig. 1: Training neural network perceptron multi-layer

first hidden layer are 1.03 and -3.81 and the four weights leading to the first hidden neuron are estimated as -3.17, -2.68, 0.25, -0.45 and 0.61 for the covariates, diameter at breast height, number of branch (primary, secondary and tertiary), total height, respectively (Fig. 1).
The generalized weights ($\widetilde{w}_i$) are given for all covariates within the same range (Fig. 1b). The distribution of the generalized weights suggests that all the covariates have effect on *Jatropha curcas* plant yield since all generalized weights are greater than zero (Fig. 1b). The synaptic weight of each covariate of the model is presented in table 2.

Models performance

Table 3 presents the values of the evaluation statistical indices for both the MLR and the ANN-MLP model. The R^2 is higher and equal to 1 for the ANN-MLP model indicating that the ANN-MLP model is more accurate. The RMSE values are very high compared to the zero value, indicating that both models have low predictive capabilities. The MLR value is negative for the MLR model and positive for the ANN-MLP model, which indicates that the MLR model underestimated the yield of the plant while the ANN-MLP model overestimated the yield of the plant (Fig. 2). Finally, the value of IA is higher for the ANN-MLP model and is close to the value one which denotes a perfect agreement between prediction and observation from the ANN-MLP model unlike the MLR model.
Fig. 2 shows the observed values of yied *Jatropha curcas* plant against the corresponding predicted models values for the *Jatropha curcas* plant trees. According to Fig. 2 and table 3, in conclusion, *Jatropha curcas* plant yield is most reliable

Table 2: Synaptic weight of each covariate (x_1 = diameter at breast height, x_2 = number of primary branch, x_3 = number of secondary branch, x_4 = number of tertiary branch, x_5 = total height)

Layer	**Synaptic weights**					
Input layer to the hidden	Intercept (a_0)	a_1	a_2	a_3	a_4	a_5
	1.03	-3.17	-2.68	0.25	-0.45	0.60
	Intercept (b_0)	b_1	b_2	b_3	b_4	b_5
	-3.81	-3.78	9.20	12.22	10.82	5.42
From hidden layer to the output layer		c_0	c_1	c_2		
		1.55	-3.22	-1.82		
Equation of output network:	$\hat{y} = g(z) = \frac{1}{1+e^{-(1.55-3.22\mu_1-1.82\mu_2)}}$					

Table 3: Performance statistics for the validation of the developed models.

Forecasting model	$\mathbf{R^2}$	**RMSE**	**MBE**	**IA**
MLR	0.55	164.84	-36.67	0.78
ANN	1.0	318.94	144.05	0.82

by using the ANN-MLP approach compared to the forecasting by using ANN models. This result may be explained by the fact that several factors affect the yield of *Jatropha curcas* plant. This complexity of factors affecting yield does not allow the ANN model to predict the yield of the plant. The relationships between the explanatory variables studied and the explained variable are not initially linear. The ANN model does not seem to be appropriate. The improvement of the predictive model with the ANN-MLP may explain the non-linearity between the variables that affect the yield of *Jatropha curcas* plant (El Badaoui et al., 2012). ANN-MLP models, as in several studies, appear to perform better than ANN models (Moustris et al., 2012; Sousa et al., 2007). The layers created in the ANN seem to take into account lost information in the case of using the ANN model. Nevertheless, the model ANN-MLP presents the difficulty of parameterization (number of neurons in the hidden layer).

Conclusion

The prediction of the yield of *Jatropha curcas* plant, based on the morphological parameters, showed that the predictive model established by the ANN-MLP method is more efficient compared to that established by the MLR-based method. This performance appears to be due to the fact that the yield of *Jatropha curcas* plant is assigned to morphological parameters by nonlinear relationships. It is important

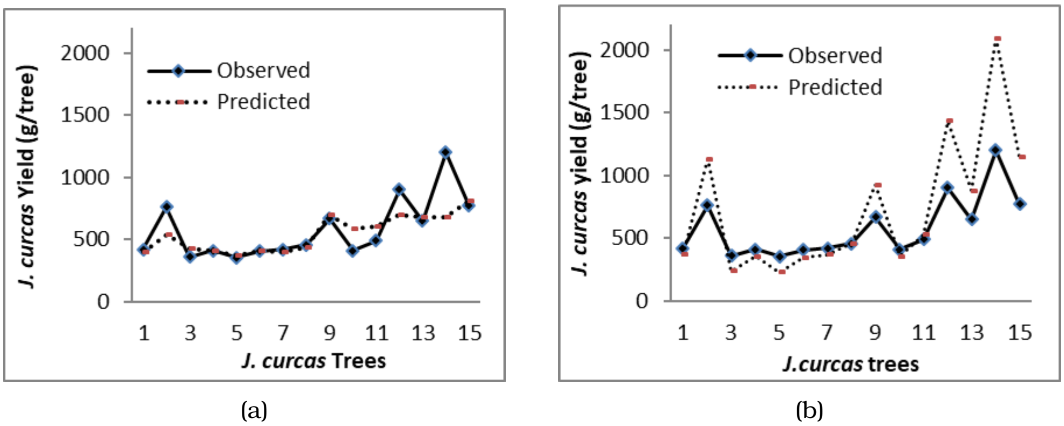


Fig. 2: Observed and predicted *Jatropha curcas* plant yield values for MLR (a) and ANN-MLP (b) model.

to continue the investigations by adding other parameters to the chosen model and also by varying the number of hidden layers.

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